Curriculum Vitae Prof. Claudio FONTANESI

Studies

Received his *degree in Chemistry, magna cum laude* (i.e. *110/110 e Lode*, the highest rank that can be achieved in the Italian academic studies), at the Dept. of Chemistry, Univ. of Modena, 15/12/1982. Thesis titled: "Theoretical study in the 1,3-Dipolar cycloaddition regioisomery", supervisor Prof. Augusto Rastelli.
PhD in Physics, University of Bath, 5 October 2017, titled "An ab-initio theoretical description of vibrational, and electronic states, in pristine and doped organic semiconductors." supervisor Dr. Enrico Da Como

Army

Under the army, Sanitary Corp, 6th Disinfection Section (Bologna), from the 15 Dec 1983 to 8 Dec 1984.

Professional Career in Industry

R&D Chemist, Ferro (ITALY), Casinalbo (MODENA), from 01 Jan 1985 to 30 May 1985.
R&D Chemist, Marazzi, Sassuolo (MODENA), from 01 Jun 1985 to 30 Apr 1987.

Academic Career

Assistant Professor of Physical Chemistry, SSD 81, UniMORE from the 01 May1987.
Associate Professor of Physical Chemistry, CHIM/02, UniMORE from the 01 Nov 2001.

Research Activity

Prof. Claudio Fontanesi research activity focuses on Physical and Molecular Electrochemistry. From a very general point of view the ultimate goal is to clarify, at a molecular level, the experimental evidence concerning the physical chemical properties of interfaces involved in electrochemical and charge transmission processes:
1) electronic properties and redox potentials relationship.
2) dynamical properties.
Interfacial Physical Chemistry: thermodynamics, kinetics and structure of the metal/solution interface, adsorption of organics (double layer capacitive measurements, adsorption isotherm fitting, 2D phase transition), Cr electrodeposition mechanism and dynamics. *Electron Transfer*: energy involved in the reduction of organics and study of the dissociative reaction path of organics. The latter based on the use of electrochemical techniques voltammetry in c.c. (linear, cyclic, chrono-methods), as well as by using Electrochemical Impedance Spectroscopy measurements. Experimental results are assessed on the basis of calculated potential energy surfaces, MD trajectories (DFT based, MPn, CI, MCSCF, DRC).
3) Spin Dependent Electrochemistry: spin filtering in electron transfer via chiral interfaces

Recent publications

[1] D. Mishra, T.Z. Markus, R. Naaman, M. Kettner, B. Gohler, H. Zacharias, N. Friedman, M. Sheves, C. Fontanesi, Spin-dependent electron transmission through bacteriorhodopsin embedded in purple membrane, **Proc. Natl. Acad. Sci.** 110 (2013) 14872–14876.

[2] P.C. Mondal, C. Fontanesi, D.H. Waldeck, R. Naaman, Field and Chirality Effects on Electrochemical Charge Transfer Rates: Spin Dependent Electrochemistry, **ACS Nano.** (2015).

[3] P.C. Mondal, N. Kantor-Uriel, S.P. Mathew, F. Tassinari, C. Fontanesi, R. Naaman, Chiral Conductive Polymers as Spin Filters, **Adv. Mater.** 27 (2015) 1924–1927.

[4] P.C. Mondal, C. Fontanesi, D.H. Waldeck, R. Naaman, Spin-Dependent Transport through Chiral Molecules Studied by Spin-Dependent Electrochemistry, **Acc. Chem. Res.** (2016).

[5] D. Di Nuzzo, C. Fontanesi, R. Jones, S. Allard, I. Dumsch, U. Scherf, E. von Hauff, S. Schumacher, E. Da Como, How intermolecular geometrical disorder affects the molecular doping of donor–acceptor copolymers, **Nat. Commun. 6 (2015)**.
[6] J. Potticary, L.R. Terry, C. Bell, A.N. Papanikolopoulos, P.C.M. Christianen, H. Engelkamp, A.M. Collins, C. Fontanesi, G. Kociok-Köhn, S. Crampin, E. Da Como, S.R. Hall, An unforeseen polymorph of coronene by the application of magnetic fields during crystal growth, **Nat. Commun.** 7 (2016) 11555.

[7] A. Kumar, E. Capua, K. Vankayala, C. Fontanesi, R. Naaman, Magnetless Device for Conducting Three-Dimensional Spin-Specific Electrochemistry, **Angew. Chem. Int. Ed.** 56 (2017) 14587–14590.

[8] L. Cigarini, D. Vanossi, F. Bondioli, C. Fontanesi, A novel synthetic strategy for magnetite-type compounds. A combined experimental and DFT-computational study, **Phys Chem Chem Phys.** 17 (2015) 20522–20529.

[9] C. Fontanesi, C.A. Bortolotti, D. Vanossi, M. Marcaccio, Dissociation Dynamics of Asymmetric Alkynyl(Aryl)Iodonium Radicals: An ab Initio DRC Approach to Predict the Surface Functionalization Selectivity, **J. Phys. Chem. A.** 115 (2011) 11715–11722.

[10] C. Fontanesi, Spin-dependent electrochemistry: A novel paradigm, **Curr. Opin. Electrochem.** 7 (2018) 36–41.

Selected publications from the past

1) C. Fontanesi, "Entropy change in the 2D phase transition of Adenine adsorbed at the Hg electrode/aqueous solution interface", ***J. Chem. Soc., Faraday Trans.***, 90 (1994) 2925.
2) C. Fontanesi, "Theoretical study of the dissociative process of the 4-chlorotoluene radical anion", ***J. Mol. Struct.*** **(THEOCHEM)**, 392 (1997) 87.
3) C. Fontanesi, "Entropy Variation in the Two-dimensional Phase Transition of Anthracene Adsorbed at the Hg Electrode/Ethylene Glycol Solution Interface." **Entropy**, 12 (2010) 570-577.

Invited Lecture and short visit invitation:

Univ. of Warsaw, Dept. of Chemistry, c/o Prof**.** Zbigniew Koczorowski**.**
Univ. of Ulm, Dept. of Chemistry, c/o Prof. Dieter M. Kolb.
ENS, Dept. of Chemistry, Paris, c/o Prof Christian Amatore.
ENS, Dept. of Chemistry, Paris, c/o Prof Damien Laage and James T. Hynes.
Univ. of Oxford, Dept. of Chemistry, c/o Prof Richard Compton.
Univ. of Aarhus, Dept. of Chemistry, c/o Prof Kim Daasbjerg and Steen Uttrup Pedersen.
TUM, Munchen, Dept. of Physics, c/o Prof. Katharina Krischer.
Univ. of Delhi, Dept of Chemistry, c/o Prof. Gurmeet Singh and Lidia Szpyrkowicz. (2010, 2011, 2015)
Univ. of Chandighar, Dept of Chemistry, c/o Prof. Gurmeet Singh and Lidia Szpyrkowicz
Univ. of Gothenburg, 1st KISS, c/o Prof. Aleksandar Matic and Prof. Bruno Scrosati.
Giornate dell'Elettrochimica Italiana (GEI 2015), Bertinoro 20 to 24 september2015.
Univ. of Milano, Dept. of Chemistry, SmartMatLab Workshop, 15 Novembre 2017. Prof. Elena Selli.
21st Int. Conf. on Solid State Ionics, 18 – 23 june 2017 Padova, Italy.
ECHEMS 12th, Milano Marittima 6th - 9th June 2017 http://sites.unimi.it/echems2017
Univ of Jerusalem, Dept. of Physics, c/o Prof. Yossi Paltiel, 22 April 2018.
Univ. of Torino, Dept of Chemistry, c/o Prof. Ornella Abollino, Dr. Agnese Giacomino, 6 nov 2018.

Long period Visiting Scientist:

Weizmann Institute of Science, Dept. of Chemical Physics, c/o Prof. Ron Naaman (2013, 2014, 2015, 2016, 2017, 2018) for a total of 15 months.

Awarded the "Joseph Meyerhoff Visiting Professorships" 2019/2020

Scientific Collaborations/Interactions

National

1) Prof. M. Innocenti. UniFI
2) Prof. Riccardo Ruffo, UniMI

International

1) Prof. Ron Naaman, Dept. of Chem. Physics, Weizmann Institute of Science, IL.
2) Dr. Enrico Da Como, Dept. Of Physics, Univ. Of Bath, UK.

Vice-President of the Electrochemistry Division, of the Italian Chemistry Society (SCI): 2011-2013

Member of the "Direttivo" of the Electrochemistry Division, Italian Society of Chemistry (SCI): 2013 - 2014

***Editor activity*:**

1) Advances in Physical Chemistry, Hindawi: http://www.hindawi.com/journals/apc/editors/
2) Guest editor: Journal of Electroanalytical Chemistry Volume 710, 1 December 2013

In charge of the following, funded, research projects:

FAR – Local Univ. of Modena – (ex 60%) 1999-2004
COFIN2000† (Interfacial structure and dynamics of electrodic processes)
CNR2000† (Charge Transfer study in electrochemistry in adsorbed auto-organized films)
COFIN2002† (Dynamics of formation of functionalized surfaces and their role in electrochemistry)
COFIN2004† (Dynamics and structural aspects of the functionalised electrode/solution interface)
PRIN2008† (A theoretical/experimental integrated study of the electrochemical processes active in direct-methanol "fuel cell").
† – Ministry National Funding assigned on a competitive basis –

Organizative Activities:

1) Local Secretary: Giornate dell'Elettrochimica Italiana, GEI 1991, Modena 16-19 settembre 1991.
2) Chairman: INCONTRI CON LE IMPRESE: Problematiche, tecnologiche e ambientali nei processi galvanici: ossidazione anodiche, elettrodeposizioni, corrosione, trattamenti superficiali. Dipartimento di Chimica, Modena 15 Giugno 2001.
3) Chairman: WORKSHOP: PERSPECTIVES IN ELECTROCHEMISTRY OF COMPLEX SYSTEMS. Dipartimento di Chimica, Centro SCS, Modena 29 Aprile 2004.
4) Chairman: Giornate dell'Elettrochimica Italiana, GEI 2010, Modena 5-10 settembre 2010.
5) Electrochemistry Delegate: XXIV Congresso Nazionale della Soc. Chim. Ital., Lecce, 11-16 Sett. 2011
6) Local Organizer Board: 8th ECHEMS 2012, Italy, (Bertinoro) june 2012.
7) ECHEMS 12th, Electrochemistry in… ingenious molecules, surfaces and devices. 6th - 9th June 2017 http://sites.unimi.it/echems2017
8) The 69th Annual Meeting of the International Society of Electrochemistry,
Electrochemistry from Knowledge to Innovation 2 to 7 September 2018, Bologna, Italy
Symposium 18: Theory: from Understanding to Optimization and Prediction

Industry Liason

1) Italtecno: 1 year research contract, 1 (6 months student bursary) 2003.
2) Ferrari S.p.A.: 1 year research contract.
3) Cromoduro: 1 borsa di studio (6 mesi) 2001.
4) Glaxo Smith Kline: 1 research contract (4 years), 1 student bursary (year), 1 Ph D funding 2003/2005.
5) BIOFER: 1 year research contract with 6 months student bursary.

Patents

1) Water splitting method and system
R Naaman, C Fontanesi, W Mtangi
US Patent App. 15/517,738

2) “SOSTANZA CHIRALE, DISPOSITIVO CHIRALE OPERANTE MEDIANTE UNA TALE SOSTANZA E USI DI UN TALE DISPOSITIVO”
Claudio Fontanesi, Mirko Gazzotti
Domanda di brevetto depositata:
Domanda numero: 102018000006874
Data di presentazione: 03/07/2018

TEACHING CAREER

At present in charge of the courses:

1) “Electrochemical Energy Conversion”, Faculty of Engineering, Univ. of Modena (D.M.270/04). Specialistic (2nd degree) Engineering Materials/Vehicle.
2) ”Physical Chemistry: Materials, Surfaces and Interphases”, compulsory for “Material Engineering Course”, Faculty of Engineering, Univ. of Modena (D.M.270/04).

Past tenure of the courses of:

1) “Lab. of Physical Chemistry 1 (for Chemistry), A.A. from 95/96 to 2006/07.
2) "Applied Phys. Chem.", (for Chemistry)
3) "Solid State Phys. Chem.”, (for Geology)
4) "Electric Measurements (A Chemistry Oriented Special Course)", for Chemistry.
5) "Molecular Electrochemistry", PhD in Chemistry
6) "Solid State Physical Chemistry", course in Geologia, Curriculum C., A.A. 2003/2004, 04/05, 05/06.
7) "Rheology Laboratory", free course Science Faculty, MM. FF. NN. A.A. from 2002/03 to 2006/07.
8) "Processi termodinamici in ambiente terrestre", course of "Scienze per l'Ambiente e il Territorio" AA 04/05.
9) "Electrical Measurements. (a Chemistry Special Course)", chemistry course, A.A.: 92/93, 93/94, 94/95
10) "Physical Chemistry", course in “Tecnologie alimentari, Facolta' di Agraria, Universita' Cattolica, Sede di Cremona”, A.A.: 98/99
11) "Physical Chemistry", course in "Scienze e Tecnologia del Packaging", Faculty of Science MM. FF. NN. University of Parma, A.A. 2006/2007.
12) "Didattica della Chimica Analitica e Laboratorio didattico di Metodologie speciali" per la classe A013 (SSIS), Facolta' di Scienze MM. FF. NN., A.A. dal 2004/2005 al 2006/2007.
11) "Physical Chemistry 1", compulsory exam for Chemistry Course, from the A.A. 2009/10.

Supervisor of 10 graduated students First/Second degree Chemistry course.
Supervisor of 23 graduated students Five Years Chemistry course.
Supervisor of 5 graduated students Second degree in Engineering (Material Eng., Vehicle Eng.)

In charge of ERASMUS exchange-project between UniMORE and University of Aarhus (DK) and TUM, *Technische Universität München*, Munchen (D).